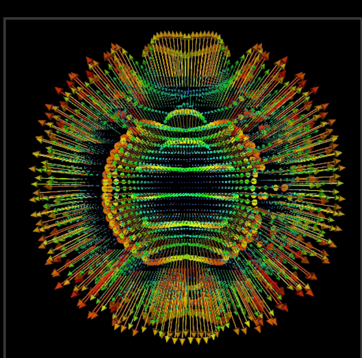
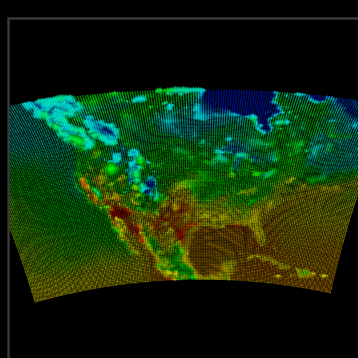
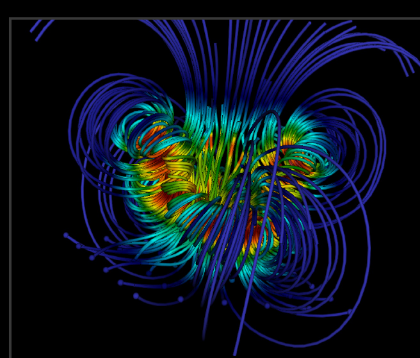
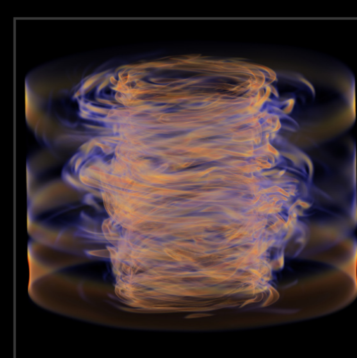
VACET

Visualization and Analytics Center for Enabling Technologies









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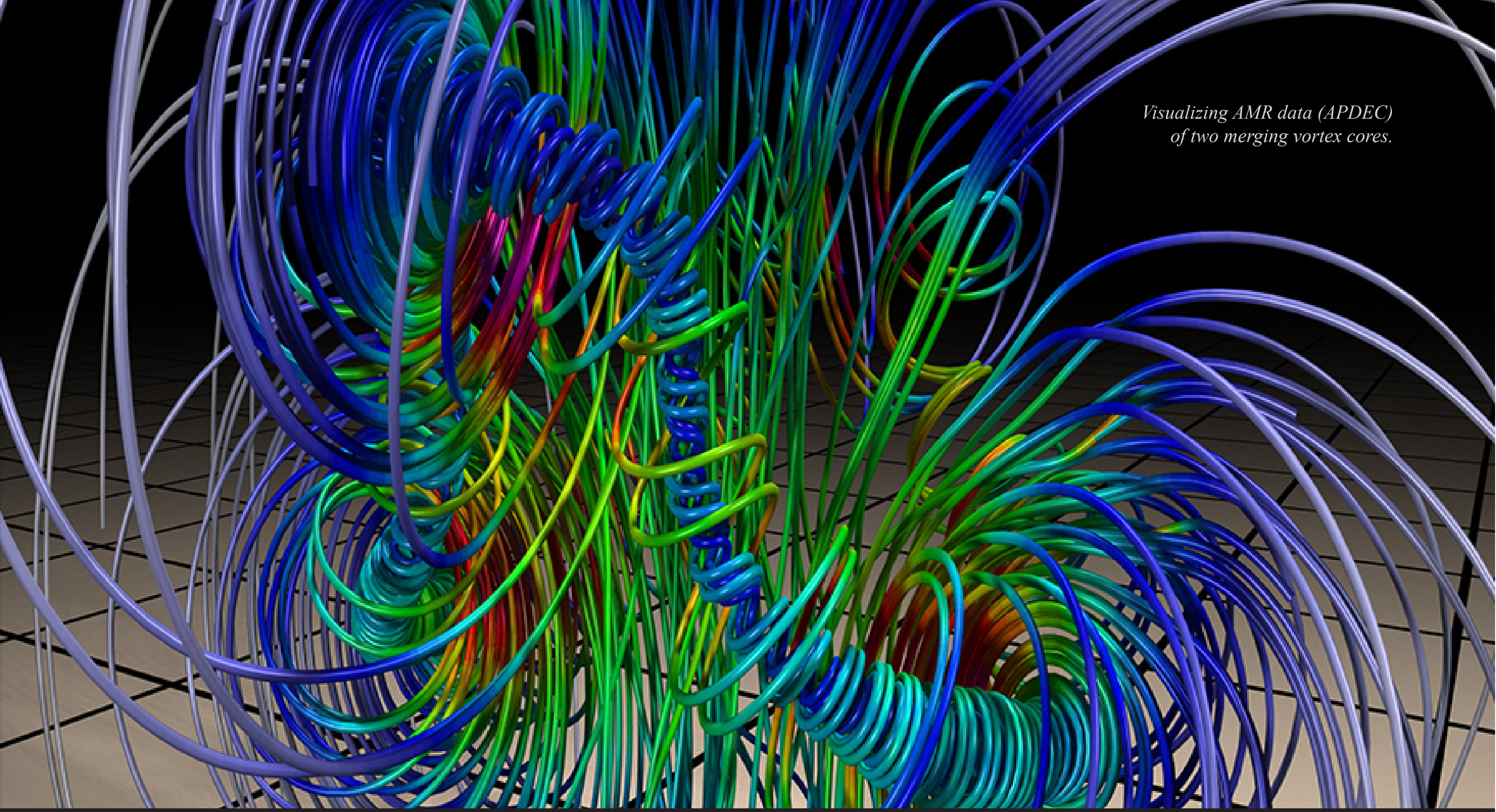

Visualizing AMR data (APDEC) of two merging vortex cores.

Visualization and Analytics Center for Enabling Technologies

The SciDAC Visualization and Analytics Center for Enabling Technologies (VACET) focuses on leveraging scientific visualization and analytics software technology as an enabling technology for increasing scientific productivity and insight. Our mission is to foster scientific insight through creating and deploying effective data understanding technology that is truly responsive to the needs of our stakeholders in the scientific research community who are "awash in data." It is widely accepted that one of the bottlenecks in contemporary science is the need to gain insight from vast collections of complex data.

The vision for our Center is to respond directly to this challenge by adapting, extending, creating when necessary and deploying visualization and data understanding technologies for our science stakeholders. Organized as a Center for Enabling Technologies, we are well positioned to be responsive to the needs of a diverse set of scientific stakeholders in a coordinated fashion using a range of visualization, mathematics, statistics, computer and computational science and data management technologies.

We are pleased to report accomplishments during the period of April 2008 through September 2008, both in terms of impact for scientific stakeholders and in terms of providing leadership in the visualization and analysis community.

VACET has made a substantial impact on the SciDAC community:

• **Accelerator Modeling.** Our research has resulted in two major capabilities needed by accelerator scientists. First, we combined forces with researchers from the SciDAC SDM Center to implement high-performance query-driven visual data analysis in a production-quality, parallel capable software application. This capability replaces a software process that consumed hours of runtime with one that runs in seconds on the Cray XT4 at NERSC. Second, we developed a technique for automatic detection of particles undergoing wakefield acceleration. This new capability also replaces an older, manual process.

• **Adaptive Mesh Refinement (AMR) Visualization.** One significant accomplishment is that the SciDAC Applied Partial Differential Equations Center has adopted VisIt as its project-wide visual data analysis software application. Additionally, CCSE researchers, who are providing the simulation code to the SciDAC Community Astrophysics Consortium, have declared that VisIt is the visualization application its researchers should use. Therefore, VACET has achieved one of its primary mission objects: provide production-quality, parallel capable AMR visualization software to the DOE scientific community. This accomplishment helps to realize

the vision for SciDAC: software infrastructure to effectively make use of parallel computing platforms for scientific knowledge discovery. Other accomplishments include: (1) performance optimizations so that time required for visualization operations on a reference APDEC dataset have been reduced by an order of magnitude; (2) support for "mapped AMR grids" are part of VisIt's production release.

• **Climate.** Our team is working with the SciDAC Science Application "Design and Testing of a Global Cloud-Resolving Model" to: (1) achieve high levels of I/O performance on the Cray XT4 system at NERSC; (2) design and implement an effective, multi-resolution data model; (3) develop and deploy the production-quality visual data analysis software infrastructure that will be used by their team. Early results have focused on testing and improving I/O performance on franklin.nersc.gov, generating early visualizations to confirm the code and data I/O layers are functioning correctly, and preliminary analysis and design of a high-performance, multi-resolution data model.

Furthermore, our team has delivered production-quality 3D visualization capabilities that are now included with the ESG's Climate Data Analysis Toolkit (CDAT). Also, our team is exploring a technology that would help streamline and improve climate data analysis workflow management with ESG researchers.

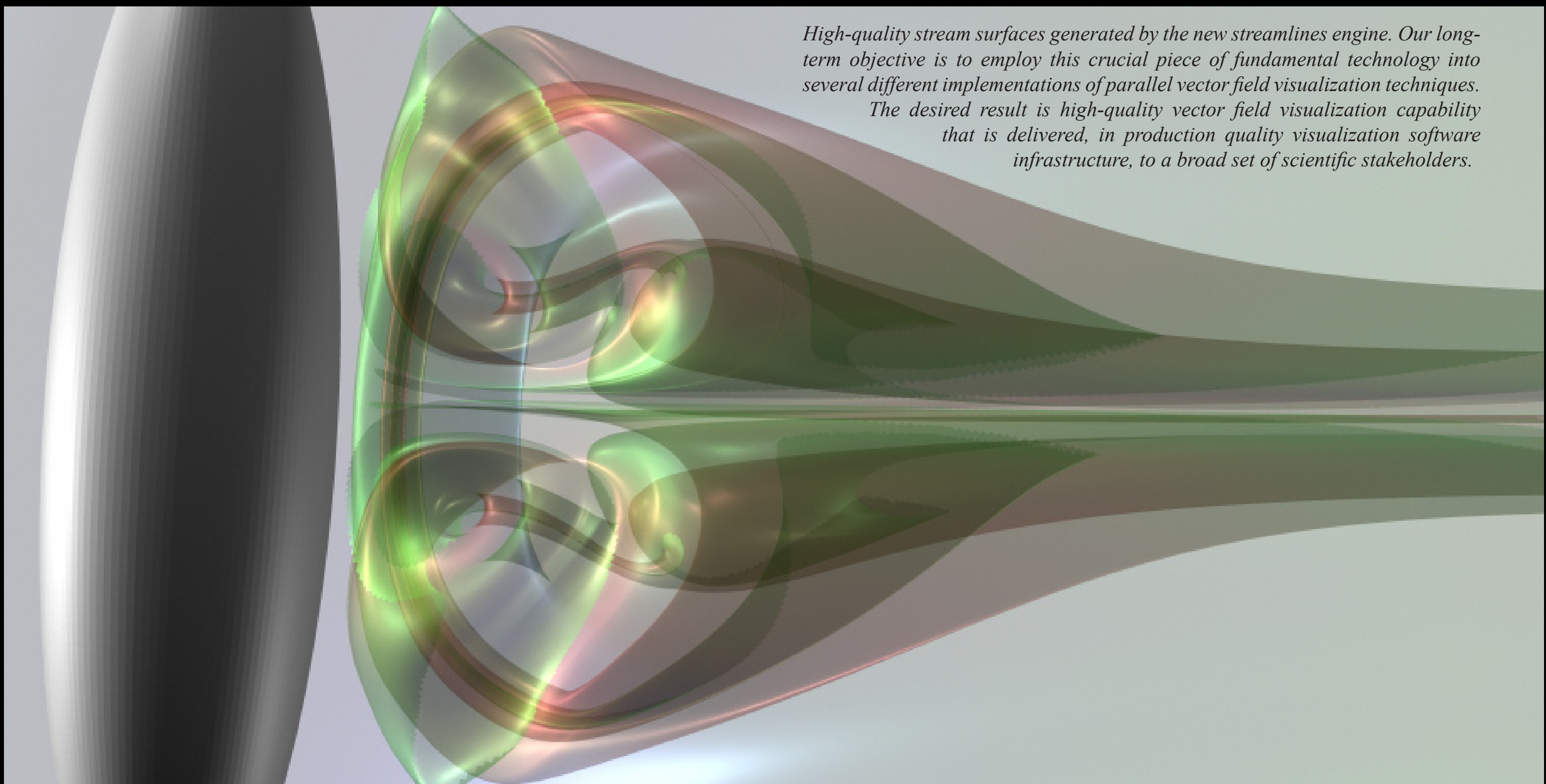
• **Combustion.** We have performed research and development of new topological analysis techniques that have proven very useful in performing quantitative analysis of large datasets produced by combustion simulations. Recent work describing topological analysis of a DNS combustion code was presented by the scientific stakeholder at the SciDAC 2008 Program Meeting. In that presentation, she indicated this new capability allowed her to see, for the first time ever, specific quantitative information about the evolution of combustion processes. This insight was not possible using traditional visualization tools (e.g., volume rendering). Related, topological analysis of AMR-based combustion models offers the first-ever insight into the relationship between the level of turbulence and its impact on the size and shape of combustion regions in a lean, premixed hydrogen flame simulation.

• **Fusion.** Our team members have been awarded a SAP project that formalizes the relationship with several different fusion projects. That work will focus on particle path and field visualization and analysis, and will leverage prior VACET work and technology applied to both Fusion and Accelerator modeling projects. Additionally, our team members have fostered a close working relationship with Tech-X Corporation with the aim of delivering a production-quality, parallel-capable visualization application for use in all Tech-X fusion and accelerator projects.

VACET continues to set the standard for visualization research productivity, outreach, and service:

• **Publications:** we report 28 peer-reviewed journal articles, 13 peer-reviewed works that appear in our field's leading conferences, several invited articles, book chapters, technical posters and technical reports.

• **Invited presentations:** we have delivered approximately



High-quality stream surfaces generated by the new streamlines engine. Our long-term objective is to employ this crucial piece of fundamental technology into several different implementations of parallel vector field visualization techniques. The desired result is high-quality vector field visualization capability that is delivered, in production quality visualization software infrastructure, to a broad set of scientific stakeholders.

twenty different invited presentations.

• **Software Tutorials:** our team has delivered five tutorials on use and application of VACET software to scientific stakeholders.

• **Workshop participation:** VACET has contributed to five different domestic and international workshops on topics ranging from high energy fusion to mathematics for petascale data.

• **Awards.** VACET wins three (of ten) "People's Choice Awards" at the SciDAC 2008 Program meeting in Seattle, WA.

• **Service.** VACET researchers have served as technical reviewer for six different journals, conferences and funding programs; and served on the Program Committee (or as general chair or co-chair) for 26 different technical conferences and symposia.

VACET also has been laying the groundwork for future results, both in terms of visualization research and in terms of deploying technology to our stakeholders:

• **Streamlines.** We have developed and deployed a parallel capable "streamlines engine" that will address needs from multiple science stakeholders (combustion, fusion, turbulence, astrophysics). This important new capability will help scientists gain deeper understanding into complex, time-varying and multi-grid vector field data produced by large-scale simulations. This work is an excellent example of VACET research, development and deployment being driven by science stakeholders' needs.

• **Embedded Boundary/Material interfaces.** Recent research has produced a highly accurate technique for computing embedded boundaries/material interfaces from simulation data containing cells with volume fraction data. The need to compute and display such interfaces is high on the priority list of one of our stakeholders, APDEC. While we have recently deployed legacy code that computes and displays embedded boundaries, we are working towards deploying the new Active Interface technique in VisIt, our production visualization application, and extending it to work with data on AMR grids.

• **High Performance Query-Driven Visualization.** As part of our research portfolio and in collaboration with the SciDAC SDM Center, we have developed a set of data structures and algorithms that show effective use of QDV on time-varying AMR datasets. In collaboration with the SDM Center and the SciDAC Institute for Ultrascale Visualization, we have developed a novel approach for indexing suitable for use on highly multithreaded, GPU platforms.

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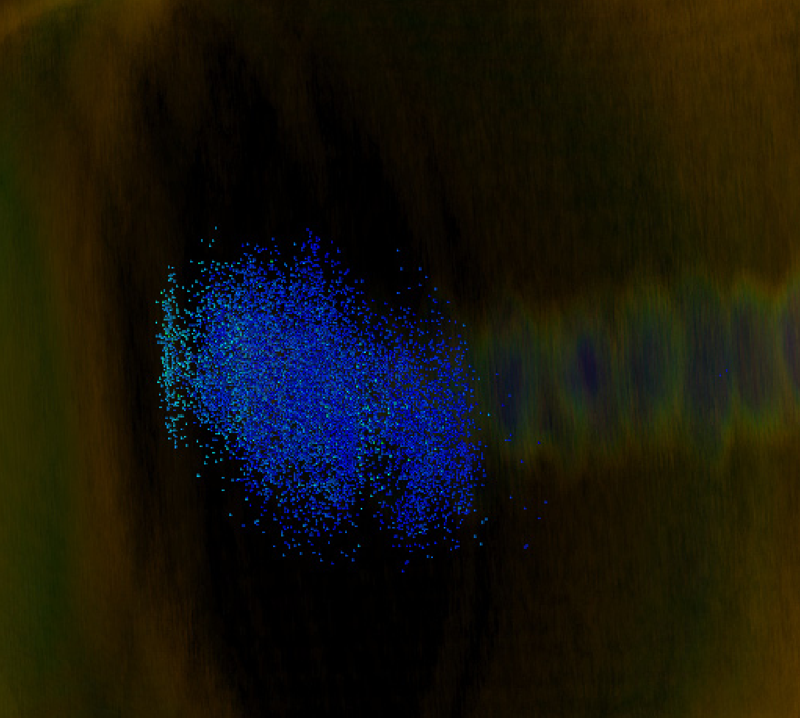


Accelerator Modeling

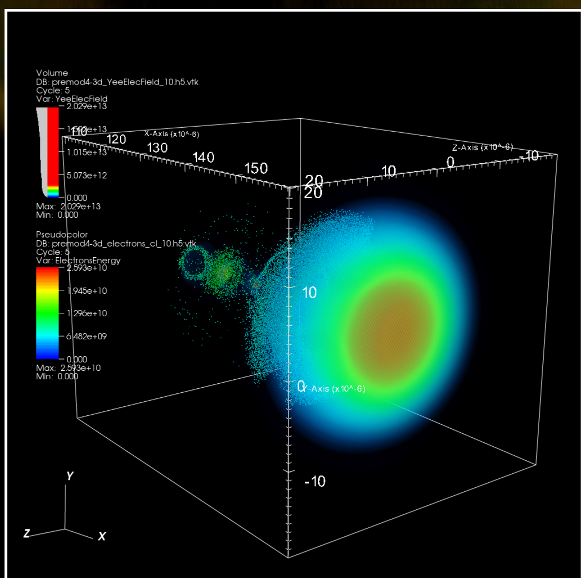
High Performance Visual Data Analysis

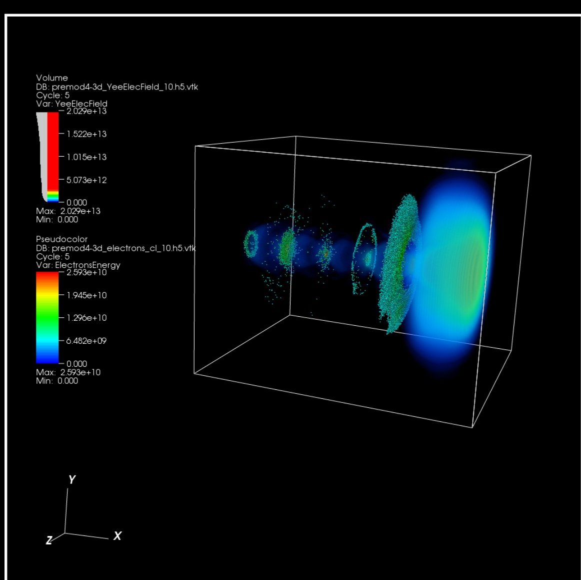
Laser wakefield simulations model the behavior of individual particles as well as the behavior of the plasma electric and magnetic fields. Output from these simulations can become quite large: today's datasets, such as the ones we study here, can grow to be on the order of 200GB per timestep, with the simulation producing approximately 100 timesteps. The scientific challenge we help address in this study is first to quickly find particles that have undergone wakefield acceleration, then trace them through time to understand acceleration dynamics, and perform both visual and quantitative analysis on the set of accelerated particles.

Our primary objective is to explore a novel technique for rapid data exploration and subsetting operations to support the types of investigatory work patterns in use by accelerator scientists. One scientific impact of our work is that we have vastly reduced the duty cycle in visual data exploration and mining. In the past, accelerator scientists would perform the "trace backwards" step using scripts that performed a search at each timestep for a set of particles. Runtimes for this operation were on the order of hours. Using our implementation, those runtimes are reduced from hours to seconds.

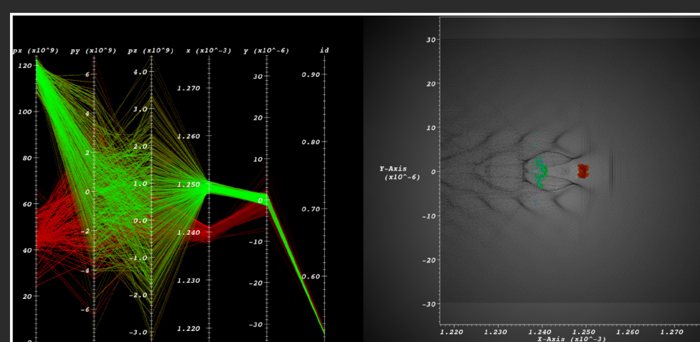
Using Analysis to Identify Beam Particles

Furthermore, we are devising a mechanism for automatically finding particles that are undergoing acceleration in a laser-wakefield simulation dataset. This capability would help to automate a process that is currently performed manually. In the long run, this capability will certainly help to accelerate data understanding. As it evolves, this technique will likely be integrated with other tools (e.g., high performance visual data analysis) as part of a broad set of HPC tools for scientific knowledge discovery in accelerator science.





Visualization using VisIt: volume rendering of the electric field and electrons rendered as particles (thresholded by the magnitude of the momentum).



Parallel coordinates and pseudocolor plot of the beam at one timestep. The context plot, shown in red, shows both beams selected by the user after applying a specific threshold. The focus plot, shown in green, indicates the first beam that is following the laser pulse. In the pseudocolor plot we show all particles in gray and the selected beams using spheres colored according to the particle's x-momentum. The focus beam is the rightmost bunch in these images. At this timestep, the particles of the first beam (green) show much higher acceleration and a much lower energy spread than the particles of the second beam.

AMR Visualization

VACET is a leader in production quality, parallel adaptive mesh refinement (AMR) visualization and analysis software infrastructure. We have recently deployed this infrastructure to our scientific stakeholders: the SciDAC Applied Partial Differential Equations Center (APDEC) and the SciDAC Community Astrophysics Consortium. This result has numerous direct benefits to those researchers. First, it allows them to "buy rather than build", thereby resulting in a direct cost savings of scientific staff: they no longer need to develop and maintain AMR visualization software. Second, the VACET technology allows them to effectively use parallel computing infrastructure to perform interactive visual data analysis to help answer scientific questions in domains like combustion and astrophysics. Third, since the VACET technologies are deployed at DOE's open computing facilities as well as on the scientists' desktop, this result is an example of successfully bridging the gap across research, development and production deployment activities within DOE's science programs.

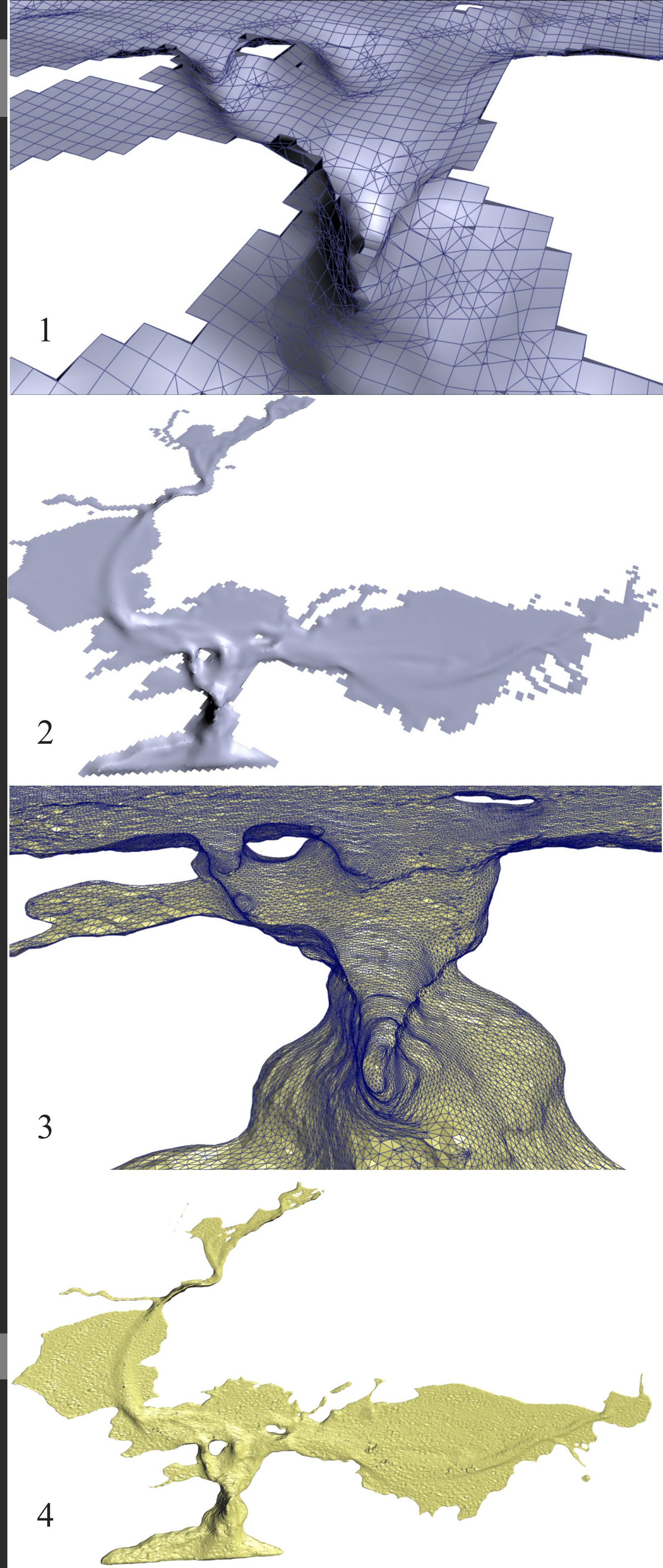
The adoption of VisIt by SciDAC stakeholders only took place because of a significant investment by VACET. This investment consisted of approximately nine months worth of effort by participants in the center employing expertise varying from performance optimization to handling of AMR data to graphical user interface design, as well as expertise with the VisIt project itself.

VACET's leadership role in AMR visualization is recognized by the broader visualization community. In 2008, VACET researchers published multiple invited papers on the subject of AMR visualization, and gave multiple invited talks at international meetings on the subject of AMR visualization.

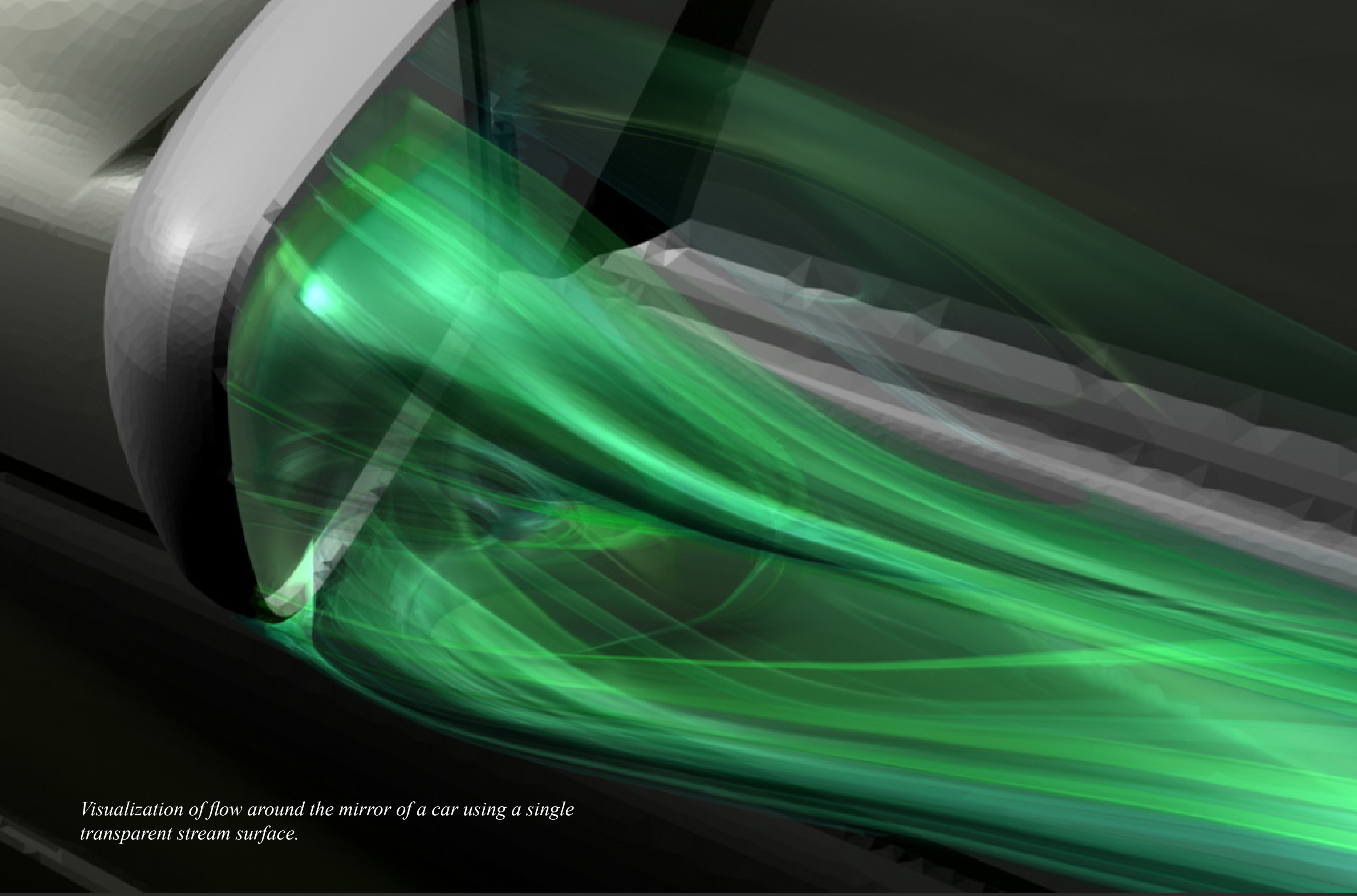
While having two major efforts within SciDAC adopt VACET technology as a "community standard" is a significant accomplishment, there is still a vast amount of work remaining. Current efforts focus on providing fundamental algorithms needed by stakeholders to enable scientific data analysis along with infrastructure enhancements aimed at easing use and production deployment.

Embedded Boundary Analysis

In many applications it is necessary to reconstruct or track the boundary surfaces, or "interfaces," between multiple materials that commonly result from multi-fluid calculations. This problem, where the generated data sets have the characteristic that each cell contains a "volume fraction" representing the percentage of each material contained in the cell, now arises in a variety of applications, and is frequently called the embedded boundary problem.



San Francisco Bay bottom comparing legacy VisIt implementation of material interfaces (1, 2) and our new material interface methods (3, 4).



Visualization of flow around the mirror of a car using a single transparent stream surface.

The challenge is to utilize the material fractions in each cell to reconstruct the boundaries between materials. VACET researchers have been developing a new approach to this problem.

Before tackling the problem, we consulted with material interface reconstruction experts from Lawrence Berkeley, Lawrence Livermore, and Los Alamos. We strove to design a broad solution that could affect many stakeholders. Various laboratories require different solutions to this problem: some require a solver that takes only general volume fractions as input and outputs material boundaries. Another requires two-material solutions on AMR meshes. All require parallel implementations and the ability to work on diverse grids.

We have developed a new solver based upon active contours. Active contours are piecewise linear curves that move toward a specific target boundary. They work by balancing three forces, a force that attempts to keep the points of the curve equidistant, a force that attempts to limit the curvature of the curve, and a volume aware force that adjusts the curve motion according to volume constraints. Once an initial approximation of the curve is generated, the active contour quickly converges to the boundary. The model works on two- and three-dimensional data sets. Initial errors for these models are very good, several orders of magnitude lower than previous methods.

Material interface reconstruction algorithms are judged by many metrics: accuracy (in terms of preserving volume fractions), smoothness of output, quality of topology, size of output (in terms of number of primitives), and, of course, execution time. We designed our algorithm to perform well with these metrics. However, we plan to demonstrate its effectiveness before moving forward. If it is successful, we will extend the algorithm for widespread use by a broad community: adapting it for use on varying grid types and extending it for use on multiple materials. After that we will productize the algorithm and deploy it within VisIt.

Parallel Streamline Infrastructure

There are several interrelated focus areas of this project. Broadly speaking, the high-level objective is to create software infrastructure for use in production-quality visual data analysis software tools that can effectively and correctly solve the vector field tracking problem in multigrid (AMR) contexts and that is suitable for use on parallel computing platforms. Several VACET team members from multiple in-

stitutions are collaborating on this effort, which is still in its early stages.

Our approach is to focus on developing a robust "streamline engine" that meets both use criteria – AMR/multigrid fields, and parallel implementation – then include this new engine into VisIt to achieve widespread use across a large base of scientific stakeholders. The AMR streamline capability was initially requested by our APDEC stakeholders, though the robust, parallel implementation will be of significant value to stakeholders in many science areas (e.g., accelerator modeling, climate, combustion, fusion, etc.).

Preliminary work to date has focused on realizing the software infrastructure for a correct unigrid solution to be run on parallel platforms. We are presently benchmarking this implementation on various parallel platforms, and performing optimizations to improve efficiency. We expect a publication to result from this effort when completed. Near-term future work will focus on realizing the multigrid/AMR implementation, and we expect additional publications from that work. Meanwhile, we continue to interact closely with stakeholders in mathematics and fusion to ensure our algorithmic development and implementation meet their scientific needs.

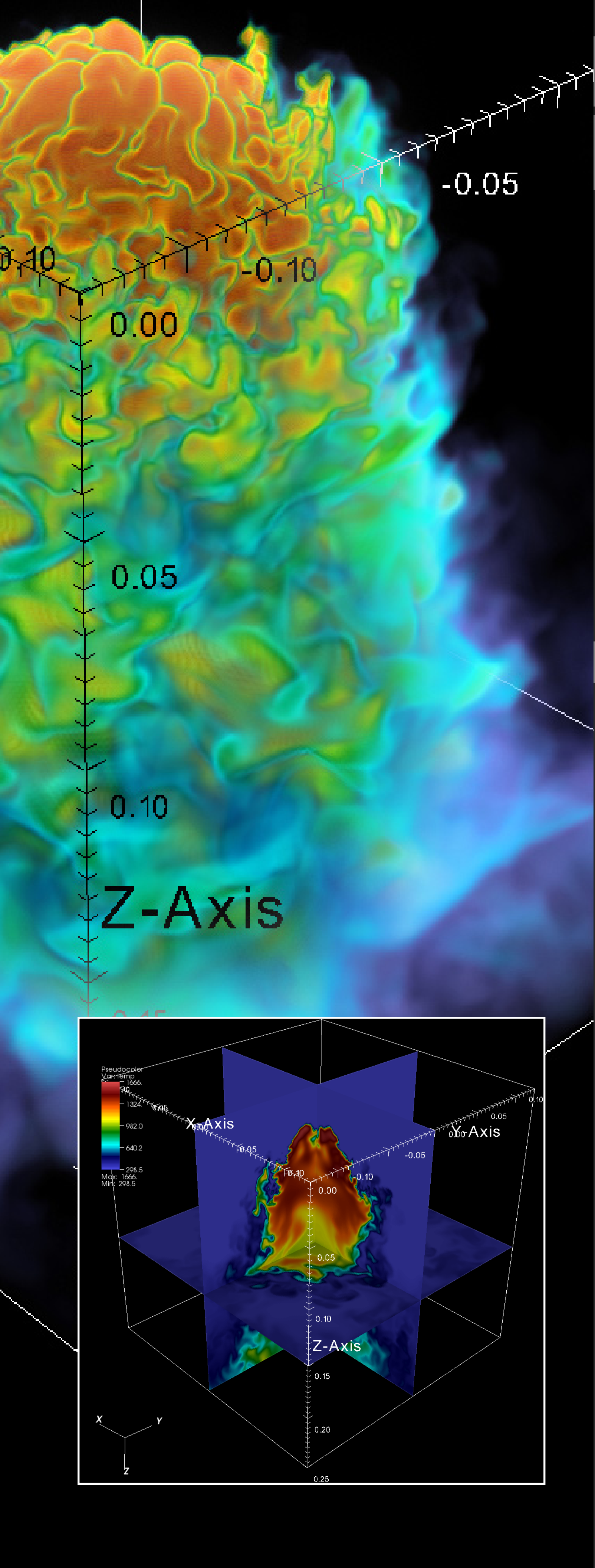
Hardware-Accelerated Volume Rendering

Although we have targeted VisIt as the production visualization tool for many of our partners, VisIt's volume rendering algorithm is below average in terms of functionality. We have decided to replace VisIt's algorithm with SLIVR: the SCIRun Library for Interactive Volume Rendering. This project, which is a long term effort involving several VACET personnel from multiple organizations, has proceeded enough to produce an early prototype (see figure 4). SLIVR offers an immediate upgrade over the functionality available in VisIt (or any production visualization tool): it contains multi-dimensional transfer functions, which allow multiple scalar quantities to affect which parts of the volume are displayed. In addition, its lighting model is a significant upgrade over what VisIt previously deployed.

This effort will have long term benefit to nearly all VACET stakeholders. It is an excellent example of transitioning research prototype technology into production use for a wide audience.

Future activities in this space (beyond productizing the deployment) focus on performance improvement, effective use on distributed memory platforms equipped with GPUs, streamlining the interfaces (user interface, software interface) between VisIt and SLIVR, and extending the fundamental SLIVR volume rendering algorithms for use on AMR grids.

Image of a tooth dataset rendered using a two-dimensional transfer function. (Inset) Snapshot of image produced by an early SLIVR/VisIt integration.



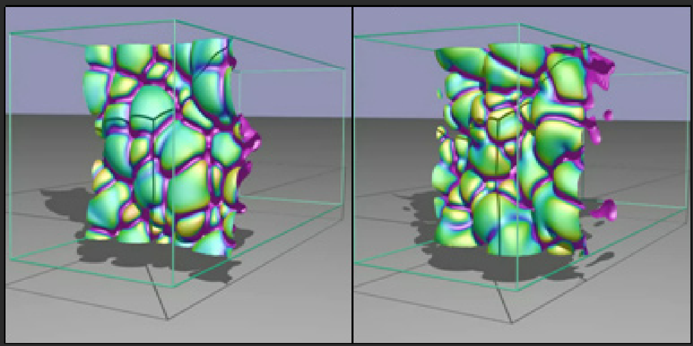
Combustion

Structural Analysis of AMR Combustion Simulation Data

Our team has been working with John Bell (LBNL) and researchers at LBNL's Center for Computational Sciences and Engineering (CCSE) to perform research, development, and application of topological analysis techniques to provide new insights into the combustion process. Bell's group works with large AMR 3D time-varying combustion simulation datasets, and needs analysis tools to aid their understanding. They are interested in formation and evolution of "extinction zones." They may be able to provide us with a Boolean volume of "burning" and "non-burning" regions, and we will perform a detailed analysis of the structural characteristics of the network of low temperature regions. They are also interested in using topological methods to identify those zones with topology-based methods. To this end we will use topological tools both feature characterization and for robust time tracking.

Quantitative Analysis of DNS Combustion Simulations

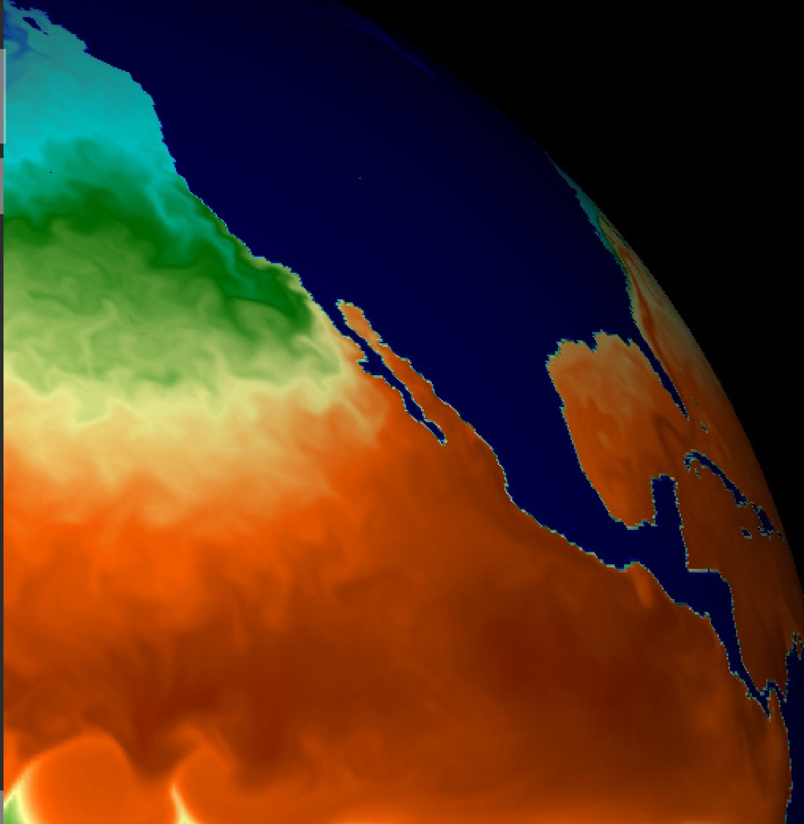
Our stakeholder, Jacqueline Chen at SNL-CA, needs to perform quantitative analysis of data produced by DNS combustion simulations to aid in the understanding of the combustion process. Our approach is to perform topological characterization of combustion features in DNS-produced data. The work has a particular focus on developing new insight about the genesis and evolution of "extinction pockets." Understanding how extinction and reignition happens in premixed hydrogen combustion allows better design of engines and power plants. We focus on the use of robust topological methods for segmentation and tracking of regions of high scalar dissipation rate that provide a good first order approximation of true extinction regions.



Above: Topological analysis provides the means for quantitative comparison of combustion region attributes in the presence of no turbulance and weak turbulence.

Left: Production quality visualization of an AMR simulation of a hydrogen flame. Sample data courtesy of J. Bell and M. Day, Center for Computational Sciences and Engineering, LBNL.

Climate

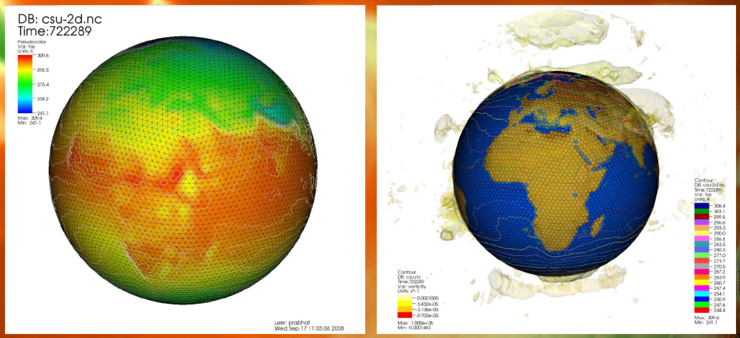


Design and Testing of a Global Cloud-Resolving Model

A collaborative effort, which includes persons from VACET and the NERSC Analytics program, is working with members of the SciDAC Science Application "Design and Testing of a Global Cloud-Resolving Model." Their objective is to run a large-scale global cloud resolving model simulation at a high level of parallelism on the Cray XT4 system at NERSC (under an INCITE award). The simulation is expected to run on 20K+ cores and dump 1TB/hr. Our work in supporting the scientists is threefold: (1) We are debugging and optimizing the collective IO performance; (2) we are providing expert advice on the data model currently being proposed for writing the simulation output; (3) we are supporting their visualization/analysis needs by writing a custom plugin in VisIt to load their data directly without the need for format conversion.

3D Visual Data Analysis in ESG's Climate Data Toolkit

The most advanced climate modeling systems seek to enable a new deeper understanding of the dynamics of global carbon cycle, atmospheric chemistry, land and ocean ecological processes and their coupling with climate. This will allow pursuing reliable answers to fundamental questions related to climate variability and global change at time scales ranging from decades to centuries. In this effort VACET is working in close collaboration with the Earth System Grid and providing new advanced data analysis and visualization tools to the CCSM Consortium and the climate modeling community in general. Our target is the deployment of a first set of tools in FY08, in time to facilitate the analysis of data for the 5th assessment report of the Intergovernmental Panel on Climate Change (IPCC).

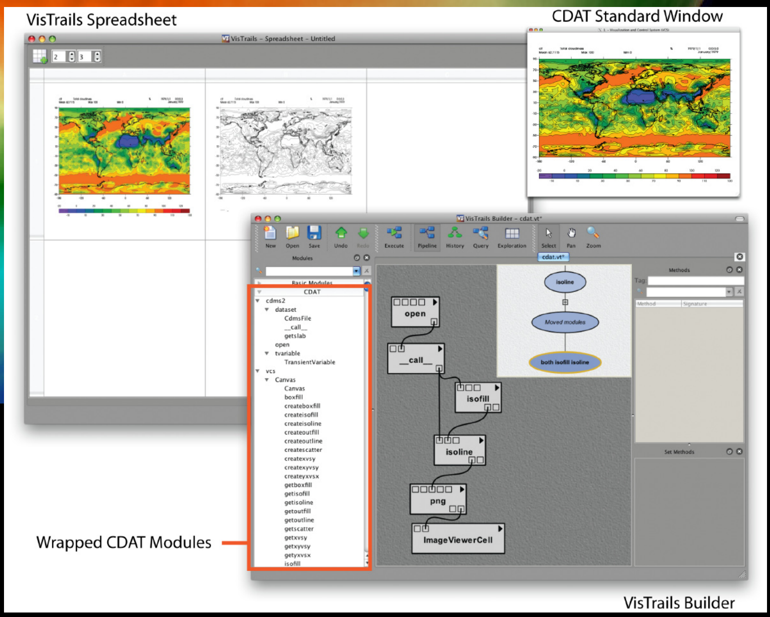


Left: VisIt plot of 2D icosahedral mesh and surface temperature. Right: VisIt plot of 3D icosahedral mesh, land cover, surface temperature and atmospheric vorticity.

Improving Workflow Efficiency in ESG's CDAT

We are integrating the Climate Data Analysis Tools (CDAT) with VisTrails as a VisTrails package. The idea is to allow the CDAT users to take advantage of the provenance mechanism as well as the visual programming interface to build CDAT workflows. The VisTrails CDAT package will contain modules for each of the CDAT subsystems (cdms, cdutil, vcs, etc.).

At this point many of the technical hurdles have been resolved, users can now create workflows and visualize the results either on the standard CDAT Window or in the VisTrails Spreadsheet as a static image. Our goal is to embed the CDAT window as a spreadsheet cell widget so users can directly interact with it.



Example of a CDAT workflow built in VisTrails. In the VisTrails builder it is shown a workflow (and its history tree) for generating a simple overlay plot using CDAT's isofill and isoline graphics methods. Notice the list of CDAT functions wrapped as VisTrails modules on the left. The results can be shown in the VisTrails Spreadsheet or in CDAT's standard window.

Fusion

Particle and Magnetic Field Visualization and Analysis

VACET is engaging with several fusion stakeholders in an effort that includes a recent SAP project (led by VACET's Allen Sanderson (Utah)).

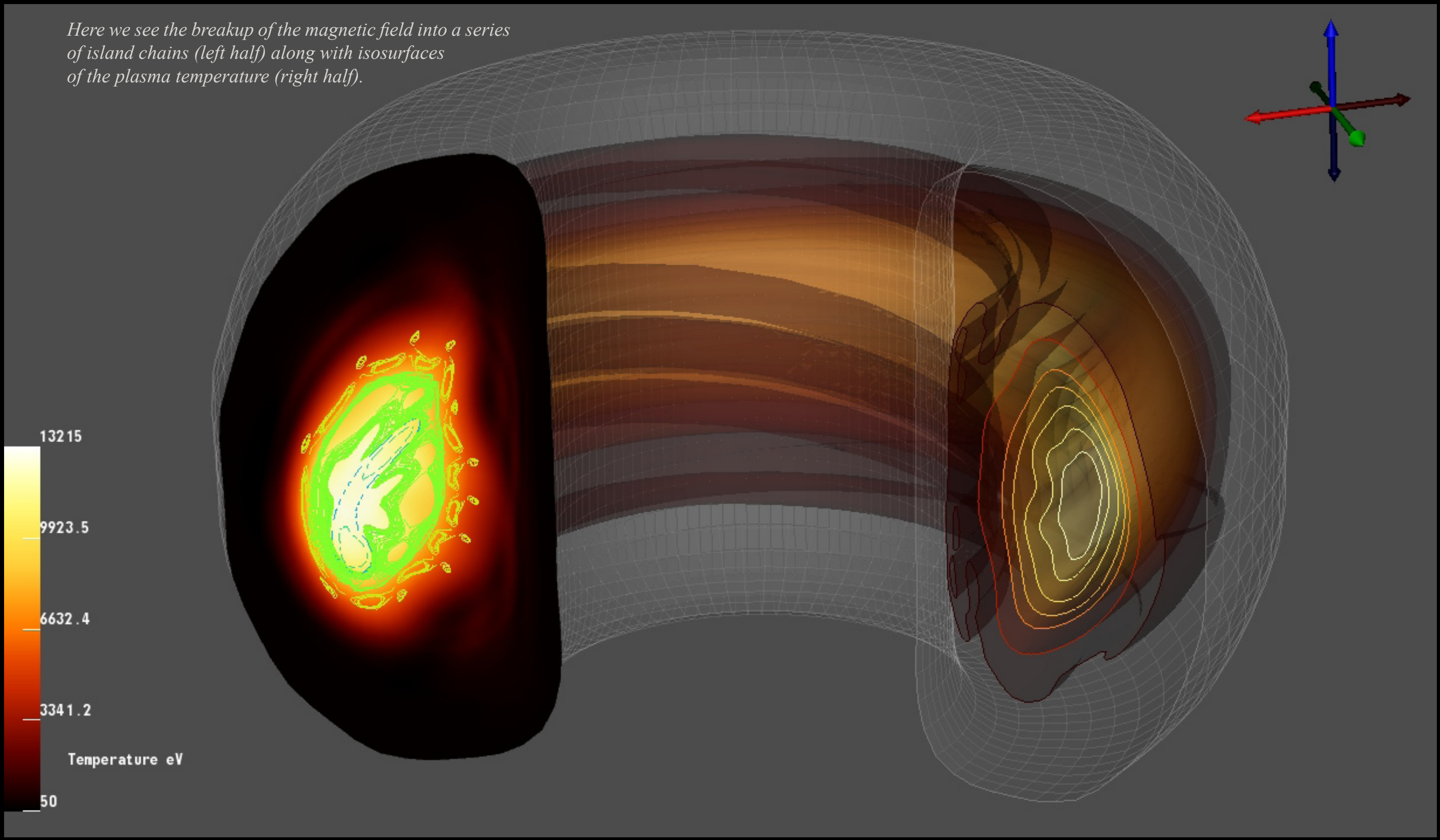
Particle Path Analysis and Visualization. The physicists are currently generating simulations that use millions to billions of particles, with each particle containing multiple scalar and vector data (multivariate data). They would like to have the ability to explore the nature of the particle orbits in an interactive manner. It is impractical to view billions, much less millions, of particles at one time and glean any insight. As such, the physicists would like to have tools that allow them cull the particles using a user defined query or other statistical tools.

At the same time as the particles are displayed, physicists are interested in seeing the particles in context of data that is not associated with the particle but is part of the simulation. This data may be scalar (electric potentials) or vector data (magnetic field) and may have its own visualization requirements. For instance, the scalar data may be viewed using a variety of techniques from volume rendering to slicing.

Magnetic Field Analysis and Visualization (in collaboration with the Fusion SAP). Physicists are currently studying the effects of magnetic islands that form in the plasma. These islands cause defects in the magnetic field and the current flow resulting in contact between previously separate regions. This contact results in "hot areas" coming into contact with "cool areas," which leads to core cooling. Physicists would like to have tools that allow them be able to automatically generate Poincaré maps of the magnetic field and detect the island formation and track them over time.

At the same time as the Poincaré maps are displayed, physicists are interested in seeing them in context of data that may or may not be associated with it, but is part of the simulation. This data may be scalar (electric potentials) or vector data (magnetic fieldlines) and may have its own visualization requirements. For instance, the scalar data may be viewed using a variety of techniques from volume rendering to slicing.

Comparative Analysis and Visualization (in collaboration with the Fusion SAP). As physicists develop and refine their simulation codes, they need tools for performing intra- and inter-simulation comparative analysis, as well as compari-



Here we see the breakup of the magnetic field into a series of island chains (left half) along with isosurfaces of the plasma temperature (right half).

son between simulations and experiments. These tools will need to be able to analyze scalar and vector data produced on different meshes and different time scales. At the same time physicists desire tools that will allow them to compare and visualize multivariate data.

Community-wide, Production Quality Visual Data Analysis Software

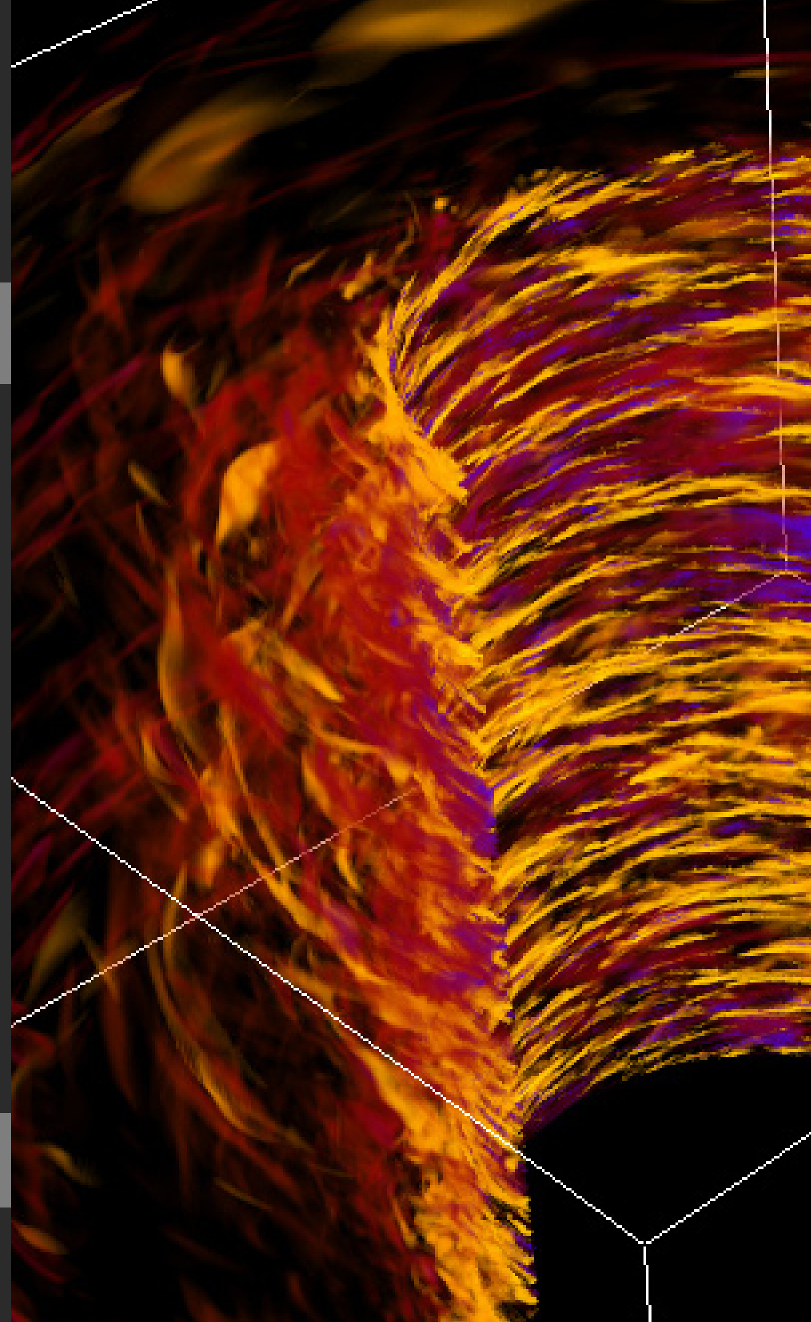
Tech-X has identified a need for production quality visualization for fusion and accelerator simulation modeling delivered within VisIt. They have several different applications and have expressed the desire to have one fully-featured tool that meets their needs for fusion and accelerator modeling projects. Due to the combination of features and performance capabilities, as well as the presence of VACET as a vehicle for developing new capabilities and providing support, they would like VisIt to be the tool of choice for their work.

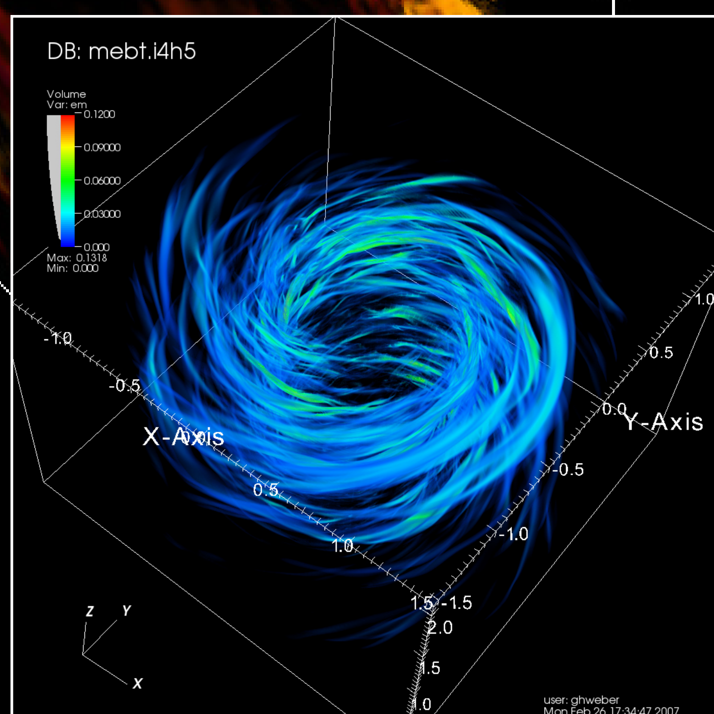
A list of milestones and deliverables was generated by Sean Ahern during a visit to Tech-X in May of 2007. Dave Pugmire visited Tech-X in January of 2008 to prioritize and clarify their needs. Dave also participated in their all hands meeting in September of 2008. In addition, Tech-X frequently makes dynamic requests, often from FACETS PI John Cary, who actively monitors the visit-developers and visit-users mailing lists.

Astrophysics

VACET's strategy for providing help to the astrophysics community focuses on teaming with the SciDAC Science Application entitled Computational Astrophysics Consortium (CAC): Supernovae, Gamma Ray Bursts and Nucleosynthesis. In a nutshell, that project combines computational and experimental science to increase an understanding of the evolution of the universe by focusing on supernovae, gamma ray bursts and nucleosynthesis.

Our approach is to undertake efforts that provide visual and data analysis infrastructure that support both aspects of this large, ambitious astrophysics project. Both the simulation and experimental communities are working together in the CAC: the experimental data provides validation of computational models, and the development of computational models helps guide how observations are performed.





Visualizing how newly born stars and black holes increase in size. In space, gases and other matter often form swirling disks around attracting central objects such as newly formed stars. The presence of magnetic fields can cause the disks to become unstable and develop turbulence, thereby causing the disk material to fall onto the central object. VACET is assisting this project by generating High-quality visualizations of data produced in these simulations. Based on these initial results, the project continues to carry out large-scale simulations to test theories on how turbulence can develop in such disks.

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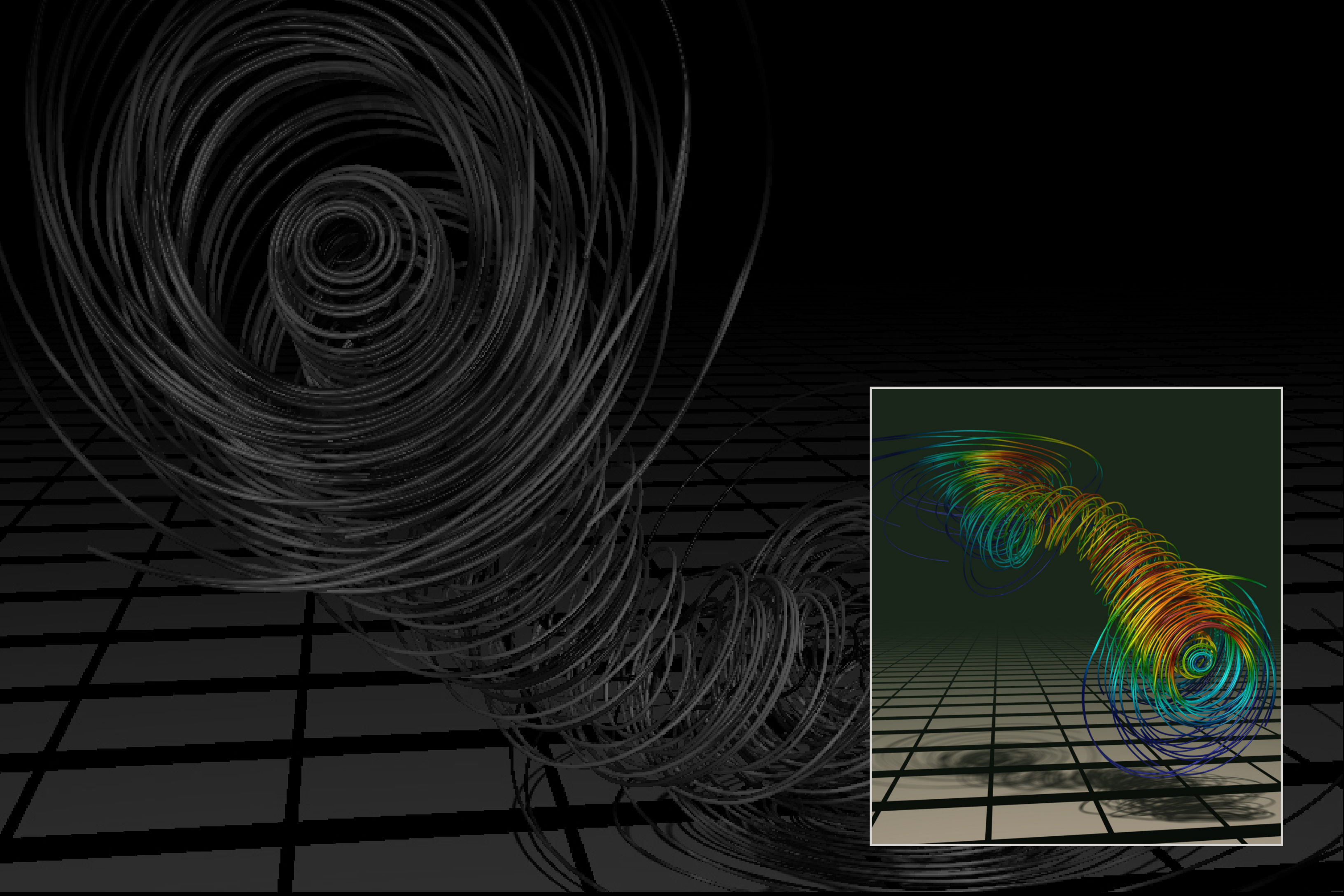
Pictured here are VACET team members and U. S. Congressman Jim Matheson at the Scientific Computing Institute, University of Utah. Left to right: V. Pascucci (LLNL), S. Ahern (ORNL), W. Bethel (LBNL), Congressman Matheson, C. Johnson (Utah), K. Joy (UC Davis).



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